

A PHYSICAL EXPLANATION FOR THE TILDE SYSTEM IN THERMO FIELD DYNAMICS

DONG MI*, HE-SHAN SONG†

Department of Physics, Dalian University of Technology, Dalian 116024,

P.R.China

YING AN

Institute of Theoretical Physics, Academia Sinica, P.O. Box 2735, Beijing

100080, P. R. China

For a two-body quantum system, any pure state can be represented by a biorthogonal expression by means of Schmidt decomposition. Using this in the composite system which include a thermodynamic system and its surroundings, it is found that the tilde system in thermo field dynamics is just the surroundings of the real system.

PACS numbers: 11.10.Wx, 05.30.-d, 03.65.Yz

In 1975, Y. Takahashi and H. Umezawa constructed a quantum field theory at finite temperature: Thermo Field Dynamics (TFD)¹. In this theory, the “fictitious” (or tilde) system is essential to convert thermal statistical average into expectation value with respect to a pure state. The central idea of TFD is the doubling of the Hilbert space of states. The operators on this doubled space are effectively doubled as well^{1,2}. After that, most of the techniques in quantum field theory can be effectively used to deal with the problems in statistical physics. However, so far there exists a question in TFD which has not been answered satisfactorily: what is the physical meaning of the tilde system? Is it really a fictitious system? The discussion of the physical meaning for the tilde system started from the birth of TFD. For example, Takahashi and Umezawa suggested in their original paper

*E-mail: dongmi@dlut.edu.cn

†E-mail: hssong@dlut.edu.cn

that the particles in the tilde system may be regarded as the holes¹. Y. X. Gui has suggested it may be regarded as the mirror world of our real one³. Before the passing away of Umezawa, he still referred to the tilde system and tried to explain its physical meaning. He pointed out that the tilde operator may be called the thermal operator for all the thermal quantities need the tilde operators⁴. We think these explanations are ambiguous and should belong to guesswork without good ground. In this letter, we first consider a two-body quantum system, its any pure state can be represented by a biorthogonal expression by means of Schmidt decomposition. Notice that any thermodynamic system is not a truly isolated system, it is always in contact with the surroundings. Using the idea about Schmidt decomposition in the composite isolated system which include a thermodynamic system and its surroundings, we find that the tilde system in thermo field dynamics is just the surroundings of the real system.

Firstly, let us imagine an isolated system with an definite state vector $|\psi\rangle$. This isolated system will be supposed a composite system and to consist of two parts. One is the system whose properties we wish to study. The remainder, to be called the surroundings of the system, will not be observed. The system to be measured has a complete set of commuting observables whose eigenvalues will be labeled collectively as a Roman letter, as i . The surroundings have a complete set of commuting observables whose eigenvalues will be labeled collectively as a Greek letter, as μ . The observables belonging to the system and surroundings commute because they refer to different things, so a basis for the isolated system, system (denoted by A) plus surroundings (denoted by B), is the set of simultaneous eigenstates⁵ $|i\rangle \otimes |\mu\rangle \equiv |i, \mu\rangle$. For simplicity, it will be assumed that all the eigenvalues are discrete, so the completeness relation is

$$\sum_{i,\mu} |i, \mu\rangle \langle i, \mu| = \hat{I}_{AB}. \quad (1)$$

By using equation (1), $|\psi\rangle$ can be expanded as

$$|\psi\rangle = \sum_{i,\mu} a_{i,\mu} |i, \mu\rangle, \quad (2)$$

with the expansion coefficients $a_{i,\mu} = \langle i, \mu | \psi \rangle$.

An observable \hat{F}_A which refers to system A alone, when considered as an observable of the composite system, should have the following form

$$\hat{F} = \hat{F}_A \otimes \hat{I}_B, \quad (3)$$

where \hat{I}_B is identity operator which acts on the Hilbert space of the surroundings. The expectation value of $\hat{F}_A \otimes \hat{I}_B$ in the state $|\psi\rangle$ is as usual

$$\langle \hat{F}_A \otimes \hat{I}_B \rangle = \langle \psi | \hat{F}_A \otimes \hat{I}_B | \psi \rangle. \quad (4)$$

With equation (2), we can write this as

$$\begin{aligned} \langle \hat{F}_A \otimes \hat{I}_B \rangle &= \sum_{j,\nu} a_{j,\nu}^* \langle j, \nu | \hat{F}_A \otimes \hat{I}_B | \sum_{i,\mu} a_{i,\mu} | i, \mu \rangle \\ &= \sum_{i,j,\mu} a_{j,\mu}^* a_{i,\mu} \langle j | \hat{F}_A | i \rangle \\ &= tr_A (\hat{\rho}_A \hat{F}_A), \end{aligned} \quad (5)$$

where

$$\begin{aligned} \hat{\rho}_A &= \sum_{i,j,\mu} a_{i,\mu} a_{j,\mu}^* | i \rangle \langle j | \\ &= tr_B (\hat{\rho}_{AB}) \end{aligned} \quad (6)$$

is called the reduced density operator (or matrix) of the system⁶.

It is easy to see that $\hat{\rho}_A$ has the following properties

$$\hat{\rho}_A^\dagger = \hat{\rho}_A, \quad (7)$$

$$tr_A \hat{\rho}_A = 1, \quad (8)$$

$$\hat{\rho}_A \text{ is semi-positive definite.} \quad (9)$$

Since the density matrix $\hat{\rho}_A$ is a semi-positive definite Hermitian matrix, it can be diagonalized and it will have non-negative real eigenvalues. Notice that the relation $\hat{\rho}_A^2 = \hat{\rho}_A$, in

general, does not hold. This means that the system is in a mixed state. Let the set $\{|i\rangle\}$ be the complete orthonormal eigenstates of the density matrix $\hat{\rho}_A$ and $\{P_i\}$ its eigenvalues ($P_i \geq 0$ since $\hat{\rho}_A$ is semi-positive definite), then the density matrix can be written in the form

$$\hat{\rho}_A = \sum_i P_i |i\rangle \langle i|. \quad (10)$$

where P_i is the probability of finding the system in state $|i\rangle$ and $\sum_i P_i = 1$. In this way, the pure state $|\psi\rangle$ of the composite system can be rewritten as the following form

$$|\psi\rangle = \sum_i P_i^{1/2} |i, \alpha_i\rangle, \quad (11)$$

where

$$|\alpha_i\rangle = \sum_\mu P_i^{-1/2} a_{i,\mu} |\mu\rangle. \quad (12)$$

Here, $\{|\alpha_i\rangle\}$ is a set of complete orthonormal states of the surroundings. In fact, equation (11) is the Schmidt decomposition of a pure state of the composite system⁷, and the set $\{|i, \alpha_i\rangle\}$ is called Schmidt basis. From the viewpoint of the surroundings B , a pure state of the composite system $(A+B)$ appears as a mixed state of the system A , described by a density matrix obtained by tracing over the degrees of freedom of the surroundings, and the density matrix $\hat{\rho}_A$ is diagonal in the Schmidt basis. That is equation (10) can also be obtained by the following way

$$\begin{aligned} \hat{\rho}_A &= tr_B (\hat{\rho}_{AB}) = tr_B (|\psi\rangle \langle \psi|) \\ &= \sum_{i,j,k} P_i^{1/2} P_j^{1/2} \langle \alpha_k | |i, \alpha_i\rangle \langle j, \alpha_j| | \alpha_k\rangle \\ &= \sum_i P_i |i\rangle \langle i|. \end{aligned} \quad (13)$$

We denote the expectation value of a quantity in mixed state by the symbol $\overline{\langle \rangle}$, for this expectation value is a double averages including the thermo and quantum averages. Thus we can express equation (5) as

$$\langle \hat{F}_A \otimes \hat{I}_B \rangle = \overline{\langle \hat{F}_A \rangle}. \quad (14)$$

Using equation (11) and (10) or (13), the above equation can be written in the Schmidt basis as

$$\sum_{i,j} P_i^{1/2} P_j^{1/2} \langle j, \alpha_j | \hat{F}_A \otimes \hat{I}_B | i, \alpha_i \rangle = \sum_i P_i \langle i | \hat{F}_A | i \rangle. \quad (15)$$

Therefore, we can see that the expectation value of a variable \hat{F}_A of the subsystem A in mixed state can be converted into the expectation value of a variable $\hat{F}_A \otimes \hat{I}_B$ of the composite system with respect to a pure state. As a result, it is inevitable to enlarge the original Hilbert space of the system to include the Hilbert space of the surroundings, and hence the corresponding degree of freedom is doubled.

Now, consider a thermodynamic system in thermal contact with a heat reservoir. We know that a macroscopic system to be dealt with in statistical physics consists of enormous number of microscopic elements interacting in a complicated fashion with the surroundings, the energy intervals between adjacent eigenstates will be much smaller than any disturbance due to the surroundings. In other words, any small disturbance will cause transitions between eigenstates, resulting in a uniform probabilistic distribution. Consequently, the behavior of the dynamic system may be expected to be described by certain probability laws⁸. This implies that the state of a system in equilibrium may be regarded as an incoherent superposition of eigenstates of the system. As is well known, a collection of identical systems used for studying probability characteristics is called an ensemble. Therefore, the states of a thermodynamic system that are described by statistical ensemble are mixed states, which are distinct from the pure states which are described by state vectors in quantum mechanics⁹. In short, owing to the uncertain interaction between the thermodynamic system and its surroundings, an uncertainty about micro-state is produced. In the way, we know only an ensemble of possible states, say $|n\rangle$, and the probabilities ρ_n of the system being in state $|n\rangle$, respectively. The information on the system is given by the density matrix.

In statistical physics we always deal with systems that interact with the surroundings. Here we can regard the system plus its surroundings as a truly isolated system. Following the former mark, we denote the thermodynamic system and its surroundings by A and B ,

respectively. Suppose \hat{F}_A is an observable of the thermodynamic system. As is well known that the thermal statistical average of this observable in the thermal equilibrium state is given by

$$\overline{\langle \hat{F}_A \rangle} = Tr \left(\hat{\rho}_A \hat{F}_A \right), \quad (16)$$

where, $\hat{\rho}_A$ is the density operator of the thermodynamic system; $Tr \left(\hat{\rho}_A \hat{F}_A \right)$ denotes the trace of the operator $\hat{\rho}_A \hat{F}_A$ and is the sum of all the diagonal matrix elements of in any representation.

For definiteness, consider now a closed thermodynamic system with the numbers of particles, volume and temperature fixed (The following discussion can be easily generalized to the open system which may be described by grand canonical ensemble.). Let \hat{H}_A be the Hamiltonian operator of the system, then the density operator of the system under consideration has the following form¹⁰

$$\hat{\rho}_A = \frac{e^{-\beta \hat{H}_A}}{Z_A}, \quad (17)$$

where

$$Z_A = Tr \left(e^{-\beta \hat{H}_A} \right) \quad (18)$$

is the partition function of the system, and $\beta = (k_B T)^{-1}$, with k_B is Boltzmann constant, T the temperature of the system.

Notice that the density operator and the Hamiltonian operator of the system commute, they possess a complete orthonormal set of simultaneous eigenstates. So, both $\hat{\rho}_A$ and \hat{H}_A are diagonal in energy representation. Assume we have the following eigenvalue equation of the Hamiltonian

$$\hat{H}_A |n\rangle = E_n |n\rangle. \quad (19)$$

A set of linearly independent eigenvectors $|n\rangle$ of \hat{H}_A can be chosen to be orthogonal and normalized

$$\langle m|n\rangle = \delta_{mn}, \quad (20)$$

and the completeness relation can be express as

$$\sum_n |n\rangle \langle n| = \hat{I}_A. \quad (21)$$

Then, the equation (17) becomes

$$\hat{\rho}_A = \sum_n \rho_n |n\rangle \langle n|, \quad (22)$$

where

$$\rho_n = \frac{e^{-\beta E_n}}{\text{Tr} e^{-\beta E_n}} \quad (23)$$

is the probability for the system to have the energy eigenvalue E_n , and it satisfies the normalization condition $\sum_n \rho_n = 1$. Thus, the thermal statistical average of the quantity \hat{F}_A can be expressed as

$$\overline{\langle \hat{F}_A \rangle} = \sum_n \rho_n \langle n | \hat{F}_A | n \rangle. \quad (24)$$

Suppose the statistical average of a quantity \hat{F}_A can be written as expectation value with respect to a pure state $|O(\beta)\rangle$. According to equation (14), we can write the following relation

$$\overline{\langle \hat{F}_A \rangle} = \langle O(\beta) | \hat{F}_A \otimes \hat{I}_B | O(\beta) \rangle. \quad (25)$$

According to equations (2), the pure state $|O(\beta)\rangle$ can be expanded as

$$|O(\beta)\rangle = \sum_{n,\mu} a_{n,\mu} |n, \mu\rangle, \quad (26)$$

where $a_{n,\mu} = \langle n, \mu | O(\beta) \rangle$, and the sets $\{|n\rangle\}$ and $\{|\mu\rangle\}$ are the complete orthonormal eigenstates of the thermodynamic system and its surroundings, respectively.

In the energy representation, by means of Schmidt decomposition, $|O(\beta)\rangle$ can be written as

$$|O(\beta)\rangle = \sum_n \rho_n^{1/2} |n, \alpha_n\rangle. \quad (27)$$

with

$$|\alpha_n\rangle = \sum_\mu \rho_n^{-1/2} a_{n,\mu} |\mu\rangle. \quad (28)$$

Obviously, the equation (25) automatically hold,

$$\sum_n \rho_n \langle n | \hat{F}_A | n \rangle \equiv \sum_{m,n} \rho_m^{1/2} \rho_n^{1/2} \langle m, \alpha_m | \hat{F}_A \otimes \hat{I}_B | n, \alpha_n \rangle. \quad (29)$$

Now, we denote α_n by \tilde{n} , the pure state $|O(\beta)\rangle$ can be written as

$$|O(\beta)\rangle = \sum_n \rho_n^{1/2} |n, \tilde{n}\rangle \quad (30)$$

where ρ_n is given by equation (23). Equation (30) is nothing but the thermal vacuum state which was introduced in thermo field dynamic by Takahashi and Umezawa¹. So, we can see clearly that the tilde system in TFD is just the surroundings of the real system.

In addition, we can see from equation (30) that the thermal vacuum state $|O(\beta)\rangle$ is an infinite superposition of the direct product state $|n\rangle \otimes |\tilde{n}\rangle$. In general, the pure state $|O(\beta)\rangle$ of the compound system cannot be expressed as a product $|n\rangle \otimes |\tilde{n}\rangle$ of pure states of its part (i. e., A and B) and hence is an entangled state¹¹. We notice that, for the system under consideration, the pure state $|O(\beta)\rangle$ is a partly entangled pure states, for the coefficients $(\rho_n)^{1/2}$ are not equal to one another. Obviously, this conclusion is true for an open system which may be described by grand canonical ensemble. In addition, for an isolated system in statistical physics (In fact, it is not a truly isolated system.), ρ_n in equation (30) becomes a constant. Since all of the expanding coefficients in equation (30) are the same now, the state $|O(\beta)\rangle$ corresponding to an isolated system is a maximally entangled state¹².

The density matrix of the compound system $(A+B)$ corresponding the state vector $|O(\beta)\rangle$ is given by

$$\hat{\rho}_{AB} = |O(\beta)\rangle_{ABAB} \langle O(\beta)| = \sum_{m,n} \rho_m^{1/2} \rho_n^{1/2} |m\rangle \otimes |\tilde{m}\rangle \langle \tilde{n}| \otimes \langle n|. \quad (31)$$

Because the $|O(\beta)\rangle$ is a pure state of the compound system $(A+B)$, the density matrix $\hat{\rho}_{AB}$ is non-diagonal. However, we are only interested in the real system A . When we measure a dynamical variable of the real system, say energy, the state of the system will transfer to one of its energy eigenstate and lead to the quantum decoherence¹³. Mathematically, this means the density matrix will be traced in the tilde states. That is we should describe the real system by means of the following reduced density matrix^{5,6}

$$\hat{\rho}_A = Tr_B(\hat{\rho}_{AB}) = \sum_l \langle \tilde{l} | \hat{\rho}_{AB} | \tilde{l} \rangle = \sum_{l,m,n} \rho_m^{1/2} \rho_n^{1/2} \langle \tilde{l} | m \rangle \otimes | \tilde{m} \rangle \langle \tilde{n} | \otimes \langle n | \tilde{l} \rangle = \sum_n \rho_n | n \rangle \langle n |, \quad (32)$$

which is the same as the corresponding one in statistical physics (see equation (22)). So, the surroundings forms an pure entangled states with the thermodynamic system upon tracing out the former we can get the correct mixed state for the latter system.

In summary, by the unavoidable interaction of the thermodynamic system in question with the surroundings, the thermodynamic system will be in a mixed state. If the thermal statistical average is replaced by a vacuum expectation value in a pure state, then the Hilbert space of the thermodynamic system should be generalized to include the one of the surroundings, and the corresponding operator become a direct product which include the operator of the system and the identity operator of the surroundings.

Acknowledgments

This project is supported by the Chinese Education Foundation(grant no. 1999014105).

[1] Y. Takahashi and H. Umezawa, *CollectivePhenomena* **2** 55 (1975).

[2] H. Umezawa, H. Matsumoto and M. Tachiki, *Thermo Field Dynamics and Condensed States*, (North-Holland, Amsterdam, 1982).

[3] Y. X. Gui, *Phys. Rev. D* **46** 1869 (1992).

- [4] *Proceedings of the 3rd Workshop on Thermal Field Theories and Their Applications*, edited by F. C. Khanna, et al, (World Scientific Publishing Co., Singapore, 1994).
- [5] J. von Neumann, *Mathematical Foundations of Quantum Mechanics*, (Princeton University Press, Princeton, 1955).
- [6] Landau, L. D., *Zeit. Phys.* **45** 430 (1927).
- [7] A. Peres, *Quantum Theory: Concepts and Methods* (Kluwer, Dordrecht, 1993).
- [8] M. Toda, R. Kubo, N. Saitô, *Statistical Physics I*, (2nd ed, Springer, Berlin, Heidelberg, 1997).
- [9] D. Landau, E. M. Lifshiz, *Statistical Mechanics*, (Pergamon, Oxford, 1958).
- [10] Kerson Huang, *Statistical Mechanics*, (2nd ed, John Wiley & Sons, New York, 1987).
- [11] E. Schrödinger, *Proc. Cambridge. Philos. Soc.* **31** 555 (1935).
- [12] S. L. Braunstein, A. Mann and M. Revzen, *Phys. Rev. Lett.* **68** 3259 (1992).
- [13] W. H. Zurek, *Physics Today* **44** 36 (1991).